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Energy band gap of β-GaN and its variation with pressure

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Abstract : A semi-empirical calculation has been carried out to find out the energy band gap of Gallium Nitride in Zinc Blende structure The normal or zero pressure lattice constant has then been used as variable parameter, and the band gap and the deformation potential has been calculated for ten values of the parameter below and above the normal lattice constant. The lattice parameter variation corresponds to pressure variation of about ±300 Kbar The band gap is not found to vary linearly, the $E_g \rightarrow a$ curve showing concavity upwards, thereby eliminating the possibility of a transition to metallic phase. The results are compared with available data from other reported works

Keywords : β-GaN, energy band gap, variation with pressure, deformation potential, phase-transition.

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The III-V nitrides *e.g.* BN, AlN and GaN have found large scale applications in laser-technology, light emitting diodes in the visible and ultraviolet region and others. In the initial stages of study, these materials were known to exist in wurtzite structure. However, the successful growth of cubic form of BN and GaN in the zinc-blende structure have led to renewed interest in the study of electronic structure and other properties of these compounds. The cBN was grown much earlier and many theoretical and experimental studies have been reported. The cubic form of GaN, known as β-GaN is still young to attract wide attention. Van Camp *et al* [1] used a local density approximation to predict its lattice constant, Bulk modulus and pressure derivative *etc.* Benkabou *et al* [2] used molecular-dynamics simulations to predict some structural and dynamical properties of the compound. Lattice constant and Bulk modulus were also reported by Lei *et al* [3], Paisley *et al* [4] and Sherwin and Drummound [5].

In the present study of β-Gan, we report the result of a semi-empirical calculation of band gap, the variation of band gap with pressure, and the deformation potential.

The calculation of band gap of β-GaN has been done semi-empirically using the general result developed by Dubey and Kumar [6] for III-V compounds, *i.e.* $\Delta E_g/\Delta \ln a$ = constant, when one moves from one compound to the other of a particular series [*e.g.* BX, AlX, GaX, InX, with X = P, As, Sb], with E_g being the band gap, and a the lattice constant. For the GaX compounds, they obtained a value 13.30 for this constant. This result is combined with the known value of lattice constant a of β-GaN as explained below.

Let E_x = Band – gap for β-GaN,

E_g = Band – gap for any of the other GaX compounds,

$\Delta \ln a = \ln a_1 - \ln a_2$.

$$\text{Hence, } 13.30 = \frac{E_x - E_g}{-(\ln a_1 - \ln a_2)}. \quad (1)$$

We have used the value 4.54 Å for lattice constant of β-GaN [4], for which

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$\ln a_1 = \ln 4.54 = 1.51293$

Let us take GaP as the other compound. Its known values are : $a = 5.45$ Å and $E_g = 2.16$ eV [7].

Hence, $\ln a_1 - \ln a_2 = \ln 4.54 - \ln 5.45$
$= -0.1827$

Therefore, $13.30 = \dfrac{E_x - 2.16}{0.1827}$

giving $E_x = 4.58$ eV.

Using known values of E_g and a for GaAs and GaSb also, the same result is obtained Thus, our semi-empirical calculation gives 4.58 eV as the band gap of β-GaN.

The effect of pressure on the band gap has been studied by treating the lattice constant as a parameter and taking ten values of this parameter, 5 each on both side of the normal value 4.54 Å, and in steps of 0.05 Å.

If a_0 and a_1 be the lattice constant (parameter) with zero pressure and pressure p respectively, then applied pressure will be given by

$$dp = B \times 3 \ln (a_1/a_0) = p, \quad (2)$$

where B = Bulk modulus of β-GaN.

The band-gap at pressure p is given in general, by

$$E_g(p) = E_g(0) + bp + cp^2, \quad (3)$$

where b and c are called the first and second order pressure coefficient of the energy difference. The hydrostatic deformation potential is given by

$$a_D = B \times [dE_g(p)/dp], \quad (4)$$

where $dE_g(p) = E_g(p) - E_g(0)$.

For studying the effect of pressure, we have used the following reported data :

$B = 1.85$ Mbar, [5]

$b = 3.58$ eV/Mbar, [1]

$c = 0.63$ eV/Mbar^2. [1]

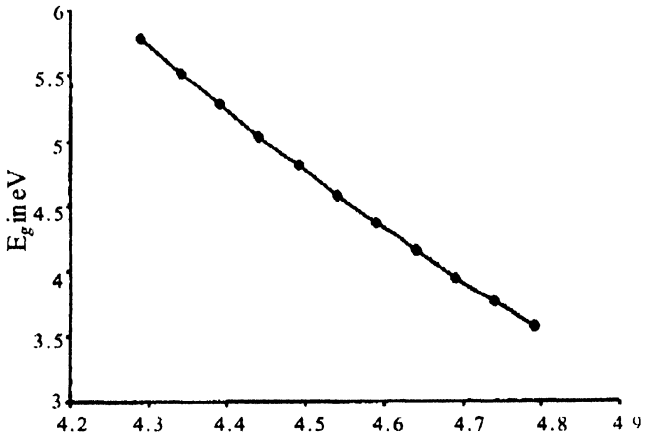
The lattice constant a has been varied from 4.29 Å to 4.79 Å (da = – 0.25 Å to + 0.25 Å) corresponding to pressure change of +0.3143 Mbar to – 0.2975 Mbar.

The deformation potentials at each pressure are calculated. The average value of $|a_D|$ is 6.63 eV. The band gaps and deformation potentials at different pressures are shown in Table 1. Figure 1 shows the variation of E_g with lattice parameter a and Figure 2 shows the variation of E_g with pressure p.

The lack of experimental and theoretical data on electronic structure of β-GaN prohibit us to present any satisfactory comparison. Though GaN in the wurtzite structure has been studied widely, workers are yet to direct their studies to its cubic form. It is generally believed that the band gap in cubic structure is less than that in wurtzite

Table 1. Variation of E_g with a and p

S. No.	a (Å)	Δa (Å)	dp (kbar)	E_g (eV)	a_D (eV)
1	4.29	–0.25	314.35	5.77	7.00
2	4.34	–0.20	250.04	5.51	6.88
3	4.39	–0.15	186.47	5.27	6.85
4	4.44	0.10	123.61	5 03	6 73
5	4 49	0 05	61 47	4 80	6 62
6	4.54	0.00	0.00	4.58	0 00
7	4 59	+0.05	–60.79	4.36	–6.70
8	4.64	+0.10	–120.92	4.16	–6.43
9	4.69	+0.15	–180 40	3 95	6 46
10	4.74	+0.20	–239.26	3 76	6.34
11	4 79	+0.25	–297.50	3.57	–6.28



Figre 1. Variation of Energy Band Gap (E_g) with lattice parameter (a)

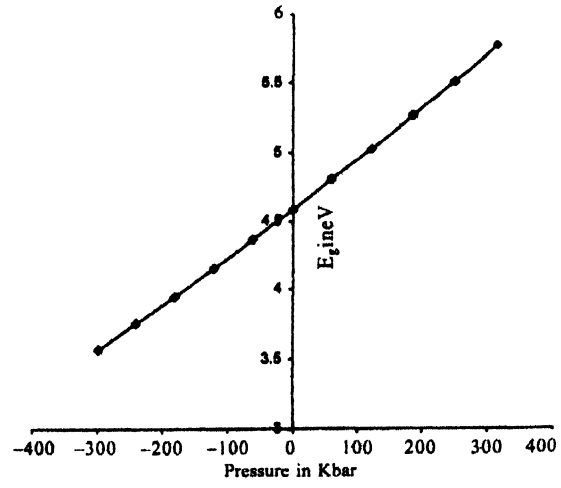


Figure 2. Variation of E_g with pressure (p).

structure. Van Vechten [8] had obtained a value of 4.8 eV for the band gap of wurtzite GaN. So our semi-empirical calculation of 4.58 eV for the gap appears to be quite reliable.

Figure 1 shows that the variation of band gap with lattice constant is not quite linear, and the curve has slight concavity upwards. This leads to the inference that transition of the semiconducting phase of β-GaN to the metallic phase may not be possible, or may occur at a very large negative pressure corresponding to large expansion of the crystal lattice.

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